1,1-dimethoxyhexan-2-one

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.05e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 7.71e-01

Nearest Neighbors from the Training Set

Image not found
Diacetone alcohol
Measured: 4.00e-12
Predicted: 6.56e-12

Image not found
2-Decanone
Measured: 1.32e-11
Predicted: 1.41e-11

Image not found
2-Nonanone
Measured: 1.22e-11
Predicted: 1.36e-11